

From Atoms to Solids II

Final Exam

Monday 22 June 2026

The exam has 2 hours duration, from 18:15 to 20:15.
(If you are eligible for extra time, the exam takes till 20:35.)

This exam has mainly questions on the content of lectures from 6 to 12.

**DO NOT START READING THE NEXT PAGES BEFORE 18:15 hrs
(when start of exam is announced)**

READ THIS FIRST

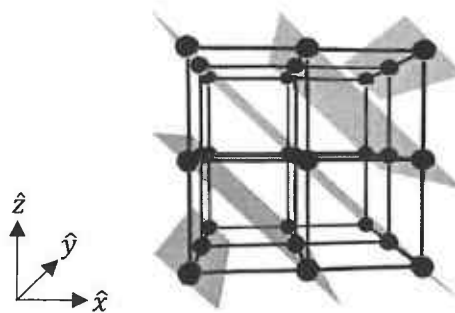
- This exam has **4** main questions with a total of 15 sub-questions, with weight points as indicated.
- Please start the answering of each main question on a new side of your papers.
- Write your name and student number on all answer sheets that you turn in.
- Clearly write the total number of pieces of paper (folded sheets) that you turn in on your first answer sheet.
- You are allowed to use a one-sided, handwritten cheat sheet (A4) that you brought yourself to the exam.
- Give clear and concise answers to the questions.
- When you are asked to make a drawing, make it large and as clear as possible.
- Make your handwriting sufficiently readable. We will not grade what we cannot read.

Natural constants and units:

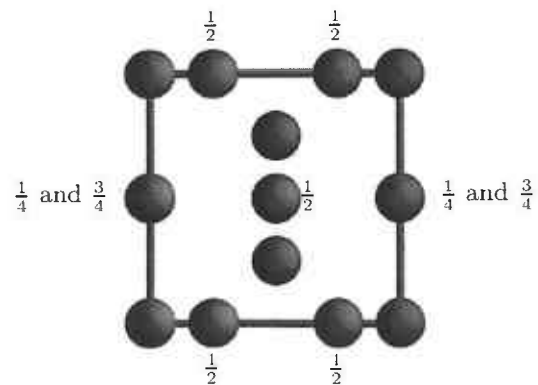
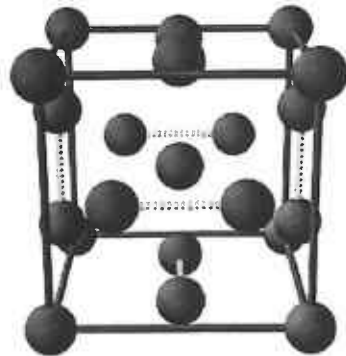
Electron mass	m_e	$= 9.109 \times 10^{-31} \text{ kg}$	
Electron charge	$-e$	$= -1.602 \times 10^{-19} \text{ C}$	
Speed of light in vacuum	c	$= 299792458 \text{ ms}^{-1}$ (exact)	
Planck's constant	h	$= 6.626 \times 10^{-34} \text{ Js}$	$= 4.136 \cdot 10^{-15} \text{ eVs}$
Planck's reduced constant	$\hbar$	$= 1.055 \times 10^{-34} \text{ Js}$	$= 6.582 \cdot 10^{-16} \text{ eVs}$
Boltzmann constant	k_B	$= 1.380649 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{ K}^{-1}$ (exact)	
Energy units	1 eV	$= 1.602 \times 10^{-19} \text{ J}$	

1: Crystal structure and waves in crystals (2+2+3+3=10pt)

- (a) Which statement about the structure factor is correct? *Only one statement is correct.*
Also write in words, in about 1-3 sentences, what the structure factor is.
- A. The structure factor depends only on the crystal's unit cell volume and X-ray wavelength.
 - B. The structure factor is maximum when the crystal has only one atom per unit cell.
 - C. The structure factor determines the angle at which diffraction occurs.
 - D. The structure factor vanishes for certain reflections due to destructive interference between scattered waves from different atoms in the unit cell.
- (b) Briefly explain the difference between the Wigner-Seitz cell and the Brillouin zone.



- (c) The figure above shows a family of lattice planes for a cubic lattice. Give the definition of a family of lattice planes and determine the Miller indices of the planes shown in the figure.



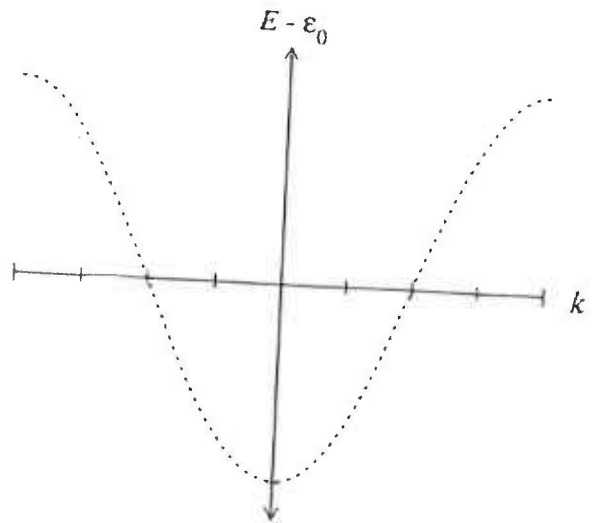
In the figures above, the cubic conventional unit cell for beta-phase fluorine is given in three-dimensional form as well as with a plan view.

- (d) Compute how many atoms are in the conventional unit cell.

2: 1D tight binding chain (6+4+2=12pt)

Consider a one-dimensional tight binding model of electrons hopping between atoms. Let the distance between atoms be called a , and here let us label the atomic orbital on atom n as $|n\rangle$ for $n = 1 \dots N$. Suppose there is an on-site energy ϵ and a hopping matrix element $-t$.

- (a) Derive the dispersion relation for electrons. (Hint: You may use the standard Schrödinger equation for a one-dimensional nearest-neighbour tight-binding chain without deriving it. Write an ansatz for ϕ_n . Assume one orbital per atom.)



Redraw the dispersion relation above, assume one orbital per atom and one valence electron per atom.

- (b) Indicate the Fermi energy in your drawing and briefly explain the position of the Fermi energy. Is the material a metal, semiconductor, or insulator? Briefly justify your answer.
- (c) In the tight-binding model, the electronic states are often approximated by a set of atomic orbitals which are assumed to form an orthonormal basis. Under what physical conditions does this orthogonality assumption break down?

3: Nearly free electron model (2+3+3+4=12pt)

- (a) Which statement about the Nearly Free Electron Model is incorrect? Only one statement is incorrect. Explain why it is incorrect in about 1-3 sentences.
- The electron wavefunctions are based on plane waves.
 - Bragg reflection plays an important role near Brillouin zone boundaries.
 - Energy gaps arise due to the periodicity of the crystal lattice.
 - The energy dispersion is parabolic throughout the entire Brillouin zone.
- (b) In the Nearly Free Electron Model, a weak periodic potential is added to free electrons. Explain why the treatment becomes problematic at the Brillouin zone boundaries and how this problem is resolved mathematically.
- (c) Make a sketch of the band structure for the Nearly Free Electron Model, with the added weak periodic potential. Make the sketch for both, in the reduced and in the extended zone scheme. Indicate parabolic regions, band gaps and Brillouin zone boundaries.
- (d) Using Bloch's theorem, show that a Bloch wave satisfies

$$\psi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{\mathbf{k}}(\mathbf{r})$$

where $\mathbf{R}$ is a lattice vector.

4: Band structures (3+2+3+4=12 pt)

- (a) Consider an energy dispersion relation for electrons in a one-dimensional crystal near the bottom of the conduction band, with the second derivative given by $\frac{\delta^2 E}{\delta k^2} = 7.0 \times 10^{-39} \text{ Jm}^2$. Assume the energy at the bottom of the conduction band is zero ($E_{min} = 0$). For this band, consider a state with $\vec{k} = 2.0 \times 10^8 \text{ m}^{-1} \hat{x}$, where $\hat{x}$ is the unit vector in the x -direction. For this electronic state, calculate the effective mass, the energy and the momentum.
- (b) An n-type semiconductor is heated from room temperature to a much higher temperature. Which of the following statements is incorrect? *Only one statement is incorrect.*
Explain why it is incorrect in about 1-3 sentences.
- A. The position of the Fermi level moves to a lower value as temperature increases.
 - B. Most donor atoms are ionized at sufficiently high temperature.
 - C. The electron and hole concentrations become approximately equal, $n \approx p \approx n_i$.
 - D. The minority carriers can no longer be neglected when determining the electrical properties of the semiconductor.
- (c) Draw a sketch of the band structures of a **direct** bandgap and an **indirect** bandgap semiconductor. Clearly illustrate the difference between these two semiconductors. Indicate the valence band, conduction band, and the band gap.
- (d) A semiconductor at room temperature (300 K) has a band gap of 1.1 eV and is n-doped such that the electron concentration is 10^{23} m^{-3} . The electron and hole effective masses are $0.25m_e$ and $0.4m_e$, respectively. Determine the hole concentration.

Hints (in the notation that was used in the book):

$$n_i^2 = \frac{1}{2} \left(\frac{k_B T}{\pi \hbar^2} \right)^3 (m_e^* m_h^*)^{\frac{3}{2}} \exp \left(-\frac{E_g}{k_B T} \right)$$

$$p = \frac{n_i^2}{n}$$